tert-Butyl alcohol 75-65-0 | DTXSID8020204

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Model	Data	

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 6.71e-01

Global applicability domain: Inside

Local applicability domain index: 6.52e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

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tert-Butyl alcohol Measured: 0.35 Predicted: 6.71e-01 Image not found

2-Methyl-2-butanol Measured: 0.89 Predicted: 1.00 Image not found

2,2-Dimethylpropanoic acid

Measured: 1.48 Predicted: 1.48

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Pentan-2-ol Measured: 1.19 Predicted: 1.21